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FAST NUMERICAL METHODS IN 3-D*

by

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I. INTRODUCTION

During the past decade, various semi-implicit finite-difference schemes such as that used in version PD2 of the Transient Reactor Analysis Code[1] (TRAC-PD2) have been applied to problems in fluid flow. The numerical method used in TRAC-PD2 is adequate for the original purpose of the code, which was analysis of large-break loss-of-coolant accidents in nuclear reactors; however, for longer term small-break transients this method is extremely inefficient. The material Courant stability limit requires time-step sizes for these transients that are much smaller than is necessary for reasonable accuracy. An obvious cure for this problem is to use a fully implicit numerical method. However, this alternative is not attractive because it requires substantial changes in the TRAC code and multiplies the cost per cell per step of the fluid-dynamics solution by a factor of six. The stability-enhancing two-step (SETS) method[2,3] was created to improve the running time of the existing TRAC code with minimal impact on the code structure and results. The SETS method eliminates the material Courant stability limit simply by adding a stabilizer step to the basic semi-implicit equations.

The SETS method implemented in the one-dimensional hydrodynamic components of version PF1 of TRAC has resulted in faster running times for systems that are modeled using only these components. For example, TRAC-PF1 performed the calculations for the Semiscale Mod-3 small-break test ~10 times faster than TRAC-PD2 (Ref. 4). Systems that include the three-dimensional vessel component generally will run somewhat faster with TRAC-PF1 because the material Courant limit is removed from the one-dimensional loop components.

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Because the use of a three-dimensional SETS method in the vessel component will allow significantly faster running times for the wide variety of transients that require multidimensional modeling, its implementation will be a major milestone in the development of reactor safety codes that run faster than real time.

II. THE SETS METHOD

To demonstrate the SETS method, we consider a simplified model for one-dimensional, single-phase flow in an unheated horizontal pipe. The differential equations for this model are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho V = 0 \quad , \tag{1}$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \rho e V = - p \nabla \cdot V \quad , \tag{2}$$

and

$$\frac{\partial V}{\partial t} + V \cdot \nabla V = - \frac{1}{\rho} \nabla p - K V |V| \quad . \tag{3}$$

Here, K is a wall friction coefficient that may be a function of velocity and fluid properties.

A staggered spatial mesh is used for the finite-difference equations; thermodynamic properties are evaluated at the cell centers and the velocity is evaluated at the cell edges. The one-dimensional difference equations are given below. To ensure stability and to maintain consistency with differencing in previous TRAC versions, flux terms at cell edges use donor-cell averages of the form,

$$\langle YV\rangle_{j+1/2} = Y_j V_{j+1/2} \quad , \quad V_{j+1/2} \geq 0 \quad ;$$

$$= Y_{j+1} V_{j+1/2} \quad , \quad V_{j+1/2} < 0 \quad . \tag{4}$$

Here, Y may be any state variable. Other forms of this average may maintain stability with higher order spatial accuracy but they have not been studied carefully. With this notation, the one-dimensional finite-difference divergence operator is

$$\nabla_j \cdot (YV) = \frac{(A_{j+1/2}\langle YV\rangle_{j+1/2} - A_{j-1/2}\langle YV\rangle_{j-1/2})}{vol_j} \quad , \tag{5}$$

where A is the area of the cell edge and vol_j is the cell volume. The term $V\nabla V$ becomes

$$V_{j+1/2}\nabla_{j+1/2}V = \frac{V_{j+1/2}(V_{j+1/2} - V_{j-1/2})}{\Delta x_{j+1/2}}, \quad V_{j+1/2} \geq 0 \quad ;$$

$$= \frac{V_{j+1/2}(V_{j+3/2} - V_{j+1/2})}{\Delta x_{j+1/2}}, \quad V_{j+1/2} < 0 \quad ; \tag{6}$$

where $\Delta x_{j+1/2} = 0.5(\Delta x_j + \Delta x_{j+1})$.

For the flow model given by Eqs. (1)-(3), the combination of basic and stabilizer equation sets can be written in several ways. One ordering that is always stable begins with the stabilizer step for the equations of motion, continues with a solution of the basic equation set for all equations, and ends with a stabilizer step for the mass and energy equations. For this ordering, the SETS finite-difference equations for Eqs. (1)-(3) are given below.

STABILIZER EQUATION OF MOTION

$$\frac{(\tilde{V}^{n+1}_{j+1/2} - V^{n}_{j+1/2})}{\Delta t} + V^{n}_{j+1/2}\nabla_{j+1/2}\tilde{V}^{n+1}$$
$$+ \beta(\tilde{V}^{n+1}_{j+1/2} - V^{n}_{j+1/2})\nabla_{j+1/2}\tilde{V}^{n}$$
$$+ \frac{1}{\langle\rho\rangle^{n}_{j+1/2}\Delta x_{j+1/2}}(P^{n}_{j+1} - P^{n}_{j})$$
$$+ K^{n}_{j+1/2}(2\tilde{V}^{n+1}_{j+1/2} - V^{n}_{j+1/2})|V^{n}_{j+1/2}| = 0 \quad , \tag{7}$$

where

$$\beta = 0, \ \nabla_{j+1/2}\tilde{V}^{n} < 0 \quad ;$$
$$= 1, \ \nabla_{j+1/2}\tilde{V}^{n} > 0 \quad .$$

BASIC EQUATIONS

$$\frac{(V^{n+1}_{j+1/2} - V^{n}_{j+1/2})}{\Delta t} + V^{n}_{j+1/2}\nabla_{j+1/2}\tilde{V}^{n+1}$$

$$+ \beta(V^{n+1}_{j+1/2} - V^{n}_{j+1/2})\nabla_{j+1/2}\tilde{V}^{n} + \frac{1}{\langle\rho\rangle^{n}_{j+1/2}\Delta x_{j+1/2}}(\tilde{p}^{n+1}_{j+1} - \tilde{p}^{n+1}_{j})$$

$$+ K^{n}_{j+1/2}(2V^{n+1}_{j+1/2} - V^{n}_{j+1/2})|V^{n}_{j+1/2}| = 0 \quad ; \qquad (8)$$

$$\frac{(\tilde{\rho}^{n+1}_{j} - \rho^{n}_{j})}{\Delta t} + \nabla_{j} \cdot (\rho^{n}V^{n+1}) = 0 \quad ; \qquad (9)$$

$$\frac{(\tilde{\rho}^{n+1}_{j}\tilde{e}^{n+1}_{j} - \rho^{n}_{j}e^{n}_{j})}{\Delta t} + \nabla_{j} \cdot (\rho^{n}e^{n}V^{n+1})$$

$$+ \tilde{p}^{n+1}_{j}\nabla_{j} \cdot (V^{n+1}) = 0 \quad . \qquad (10)$$

STABILIZER MASS AND ENERGY EQUATIONS

$$\frac{(\rho^{n+1}_{j} - \rho^{n}_{j})}{\Delta t} + \nabla_{j} \cdot (\rho^{n+1}V^{n+1}) = 0 \quad ; \qquad (11)$$

$$\frac{(\rho^{n+1}_{j}e^{n+1}_{j} - \rho^{n}_{j}e^{n}_{j})}{\Delta t} + \nabla_{j} \cdot (\rho^{n+1}e^{n+1}V^{n+1})$$

$$+ \tilde{p}^{n+1}_{j}\nabla_{j} \cdot (V^{n+1}) = 0 \quad . \qquad (12)$$

A tilde above a variable indicates that it is the result of an intermediate step, not the final value for the time step.

The material Courant stability limit is eliminated by treatment of the terms $V\nabla V$, $\nabla \cdot \rho V$, and $\nabla \cdot \rho e V$ during the two steps. Additional stability is obtained with the particular form for the friction terms and the use of nonzero values of β in the $V\nabla V$ terms. These special terms for friction and $V\nabla V$ are obtained by linearizing similar terms that are fully implicit in velocity, ($K^n_{j+1/2} V^{n+1}_{j+1/2} |V^{n+1}_{j+1/2}|$ and $V^{n+1}_{j+1/2} \nabla_{j+1/2} V^{n+1}$).

Equation (7), which represents a tridiagonal linear system in the unknown $\tilde{V}^{n+1}$, is solved first. Next, the coupled nonlinear system given by Eqs. (8)-(10) is solved. In practice this is accomplished by a Newton iteration in which the linearized equations are reduced to a linear system involving only pressure variations (Ref. 4). Once these equations are solved, V^{n+1} is known; hence, Eqs. (11) and (12) are simple tridiagonal linear systems, with unknowns ρ^{n+1}_j and $\rho^{n+1}_j e^{n+1}_j$, respectively.

When this equation set is adapted to flow in complex piping networks or to multidimensional problems, the pure tridiagonal structure is lost; however, the matrices are still sparse. Reference 2 describes the extension of the SETS method to two-phase flow.

III. EXTENSION OF SETS TO 3-D

The computational feasibility of a three-dimensional SETS method first was demonstrated by the development of a new hydrodynamics code, SETS3D, which modeled the three-dimensional flow of an ideal gas. The extension of the SETS method to three-dimensional flow is straightforward except for the equation of motion. We found that the stabilizer equation of motion may be replaced by three equations for the three velocity components; that is, the coupling among the difference velocity components from the cross-derivative expressions in the momentum flux terms of these equations may be treated explicitly.

The seven-point, finite-difference approximation used in the various convective terms of the three-dimensional SETS formulation results in several large, sparse, banded matrices of the order of the number of hydrodynamic cells. Direct solution of these large sparse matrices is expensive and inefficient both from the standpoint of computational cost and of computer storage. These matrices may be solved efficiently through the use of specialized routines for banded linear systems such as those developed for the Cray-1 by Tom Jordan of the Computer Research and Applications Group at Los Alamos or by the use of iterative methods.[5]

The stability of the SETS formulation in SETS3D was tested by running a number of different two- and three-dimensional flow problems until steady state was achieved with the maximum time step fixed at the material Courant limit and again with the maximum time step allowed to increase arbitrarily. In all cases studied, the steady states were maintained at the largest time steps.

Following the successful tests of the original version of SETS3D, the code was extended to handle a second phase. The stability of the formulation again was tested as described above, using a variety of two-phase, air-water problems. Stability was maintained at the highest Courant number tested, that is, 40,000. Appendix A describes the two-phase SETS3D code.

IV. CONCLUSION

The SETS method has been extended successfully to equations for three-dimensional, two-phase flow and the demonstration computer code used for this extension has been written in a form that can be adapted by other researchers. The method currently is being incorporated into our reactor safety systems code to provide the numerical foundation for a multidimensional code that can run faster than real time. We expect that SETS will be very useful for a wide range of multiphase and reacting flow problems where first-order-accurate difference methods are appropriate.

APPENDIX A

SETS3D CODE DESCRIPTION

We have developed a new hydrodynamics code, SETS3D, to provide a test-bed for multidimensional versions of SETS. This code models three-dimensional, two-phase flow with the SETS method as well as with the standard semi-implicit method used in TRAC-PF1. The flow geometry, specified in Cartesian or cylindrical coordinates, is constrained to a regular grid for solution of the finite-difference equations. Constant velocity or constant pressure boundary conditions are specified independently through input at each of the external cell faces.

Structures within the flow vessel are handled the same way as in TRAC-PF1; that is, a flow-volume fraction is input for each hydrodynamic cell and a flow-area fraction is input for each cell face of the staggered spatial grid. These fractions then are used to scale the geometric volumes and areas of the grid. Structures that can act as flow straighteners may be added through input for each cell face. A flow straightener causes flow normal to the face; that is, flow through the face cannot contribute to a cross term in the velocity equations.

The fluid material properties in SETS3D are defined by the TRAC thermodynamic routines. The liquid phase is water and the vapor phase is a steam-air mixture where the air partial pressure may be zero. The present version of SETS3D does not contain a constitutive package; that is, there are no models for such factors as wall shear, interfacial shear, structure-to-fluid heat-transfer coefficients, nor for terms describing processes such as boiling. These parameters currently are defined by input or are set to constant values in the code. However, because the SETS3D code is modular, a variety of constitutive packages could be added and tested easily.

The TRAC-PF1 data base is structured dynamically using pointers; that is, the variables of a given data type, such as cell-centered pressures or face-centered flow areas, are stored contiguously. The pointers define the address of the starting location for each data type. A pointer must be defined for each data type. We have discovered through experience that this type of data structure is difficult to maintain, inflexible, and cumbersome in a number of ways. The SETS3D data base has been inverted so that all of the data for a single hydrodynamic cell are stored contiguously. The structure of this data base may be defined by a single parameter, the number of data types. Our experience with SETS3D has shown that code development is easier and quicker with this inverted data base and the code structure is more efficient.

We plan to make a single-phase version of SETS3D available to interested researchers. The following code features have been added to increase the utility of the code. The ~8000 lines of FORTRAN source code are maintained using the commercially available utility Historian, which is similar to the CDC Update utility. The code includes extensive comments regarding both data structure and computational flow. The structure of this version will not allow it to be incorporated into TRAC.

The SETS3D code was developed for use on a Cray-1 computer. All of the hydrodynamic loops have been written so as to vectorize. Vectorization compatibility was built into the initial code design because we have discovered that it is difficult to restructure existing codes so that they will vectorize. For example, it is expensive to vectorize logical branches. In the case of the boundary conditions, logical branches were avoided by increasing the size of the computational grid so that the boundary values could be stored and referenced directly. The extra terms in the cylindrical forms of the velocity equations were coded with additional factors that are defined as zero when the input is specified in Cartesian coordinates. Processes that could not be vectorized easily were coded in separate loops from those that could be vectorized.

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